A whirlwind tour of scikit-learn

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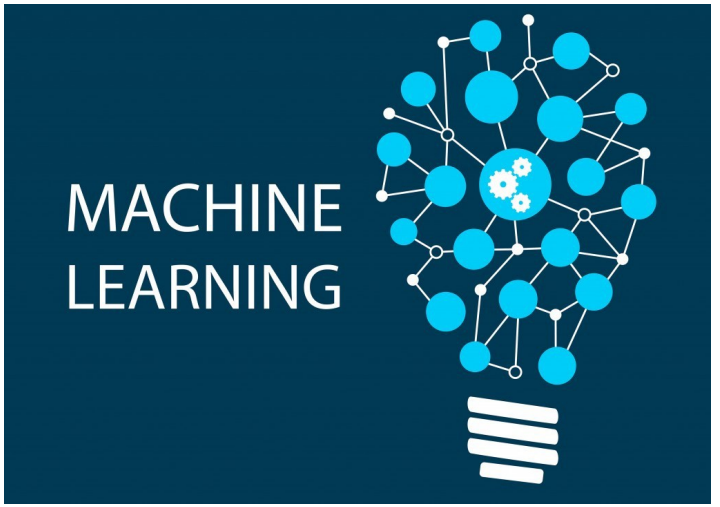
What is scikit-learn?


python


MACHINE
LEARNING

Mission

Commoditize and Democratize Machine Learning

Classification
Regression
Clustering
Semi-Supervised Learning
Feature Selection
Feature Extraction
Manifold Learning
Dimensionality Reduction
Kernel Approximation
Hyperparameter Optimization
Evaluation Metrics
Out-of-core learning
……

okc

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Basic API

Representing Data

one sample

$$X = \begin{pmatrix} 1.1 & 2.2 & 3.4 & 5.6 & 1.0 \\ 6.7 & 0.5 & 0.4 & 2.6 & 1.6 \\ 2.4 & 9.3 & 7.3 & 6.4 & 2.8 \\ 1.5 & 0.0 & 4.3 & 8.3 & 3.4 \\ 0.5 & 3.5 & 8.1 & 3.6 & 4.6 \\ 5.1 & 9.7 & 3.5 & 7.9 & 5.1 \\ 3.7 & 7.8 & 2.6 & 3.2 & 6.3 \end{pmatrix}$$

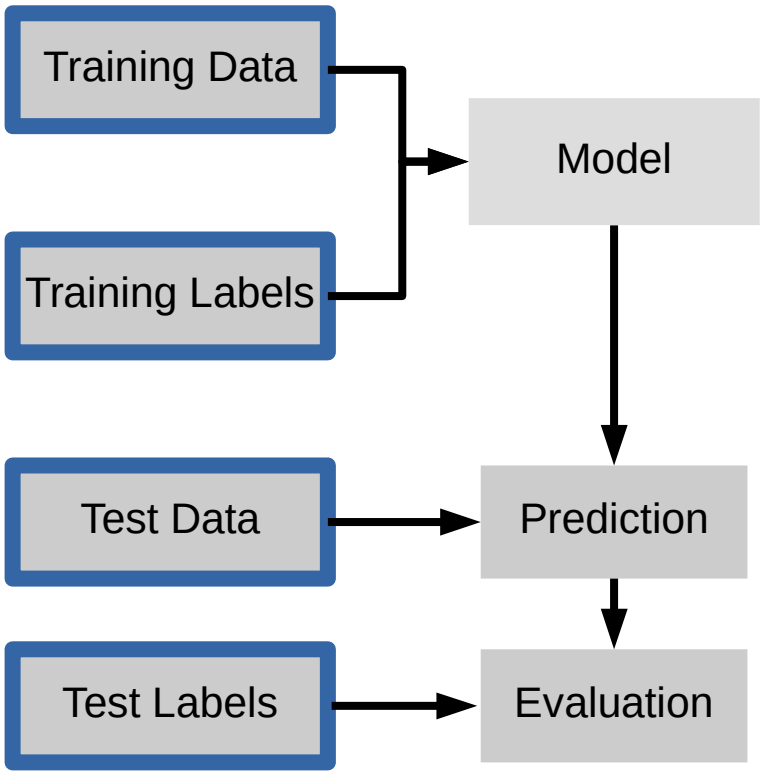
one feature

$$y = \begin{pmatrix} 1.6 \\ 2.7 \\ 4.4 \\ 0.5 \\ 0.2 \\ 5.6 \\ 6.7 \end{pmatrix}$$

outputs / labels

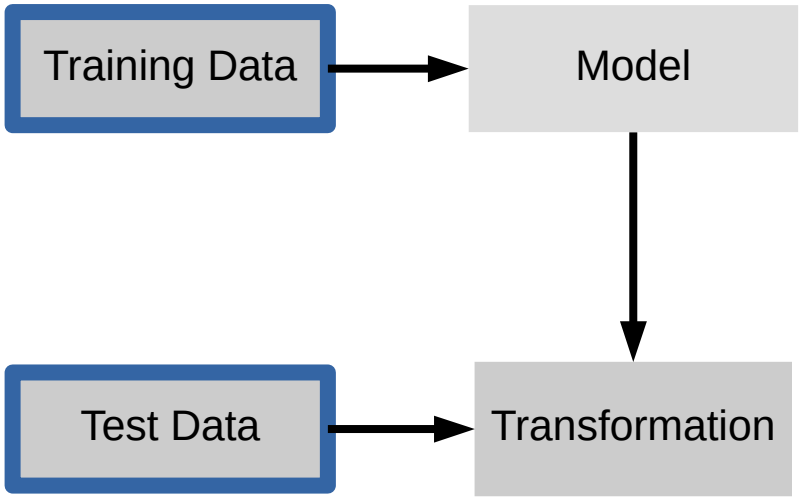
```
clf = RandomForestClassifier()

clf.fit(X_train, y_train)
```

```
y_pred = clf.predict(X_test)

clf.score(X_test, y_test)
```



Unsupervised Transformations

```
pca = PCA()

pca.fit(X_train)

X_new = pca.transform(X_test)
```

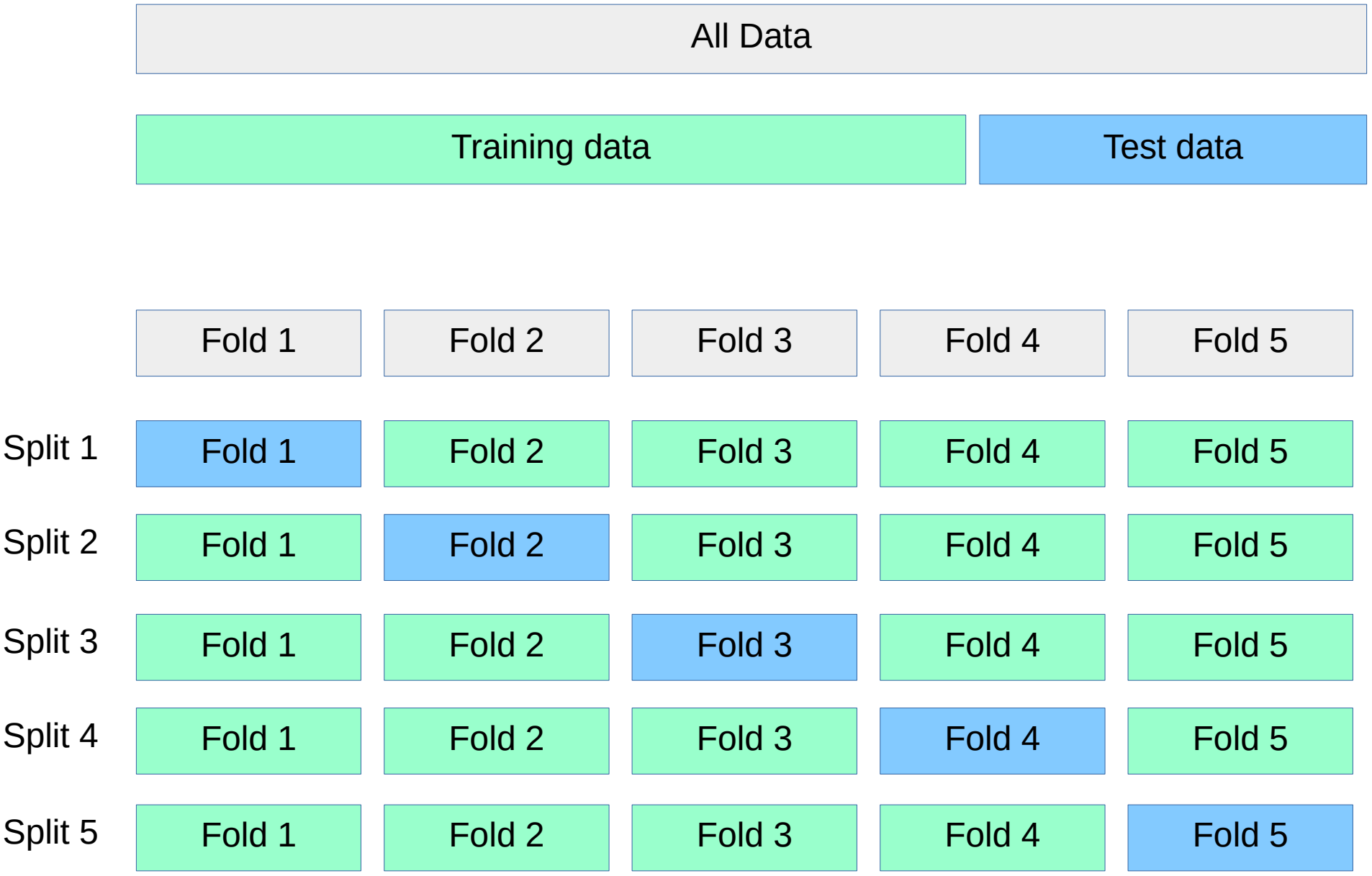


Core API Summary

`estimator.fit(X, [y])`

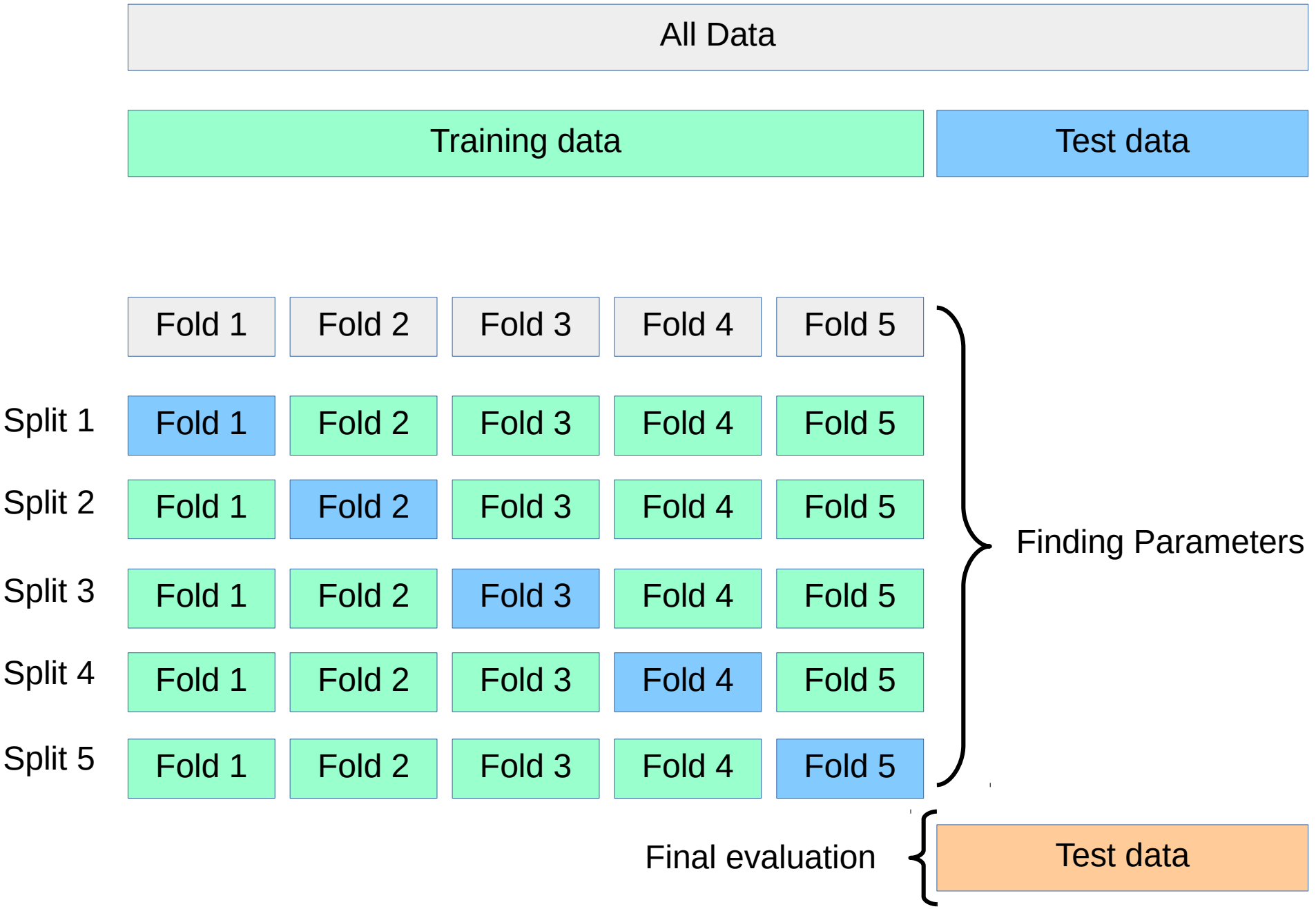
`estimator.predict`	**`estimator.transform`**
Classification	Preprocessing
Regression	Dimensionality reduction
Clustering	Feature selection
	Feature extraction

Model Evaluation and Model Selection


All Data
Training data
Test data
Fold 1
Fold 2
Fold 3
Fold 4
Fold 5
Split 1
Fold 1
Fold 2
Fold 3
Fold 4
Fold 5
Split 2
Fold 1
Fold 2
Fold 3
Fold 4
Fold 5
Split 3
Fold 1
Fold 2
Fold 3
Fold 4
Fold 5
Split 4
Fold 1
Fold 2
Fold 3
Fold 4
Fold 5
Split 5
Fold 1
Fold 2
Fold 3
Fold 4
Fold 5

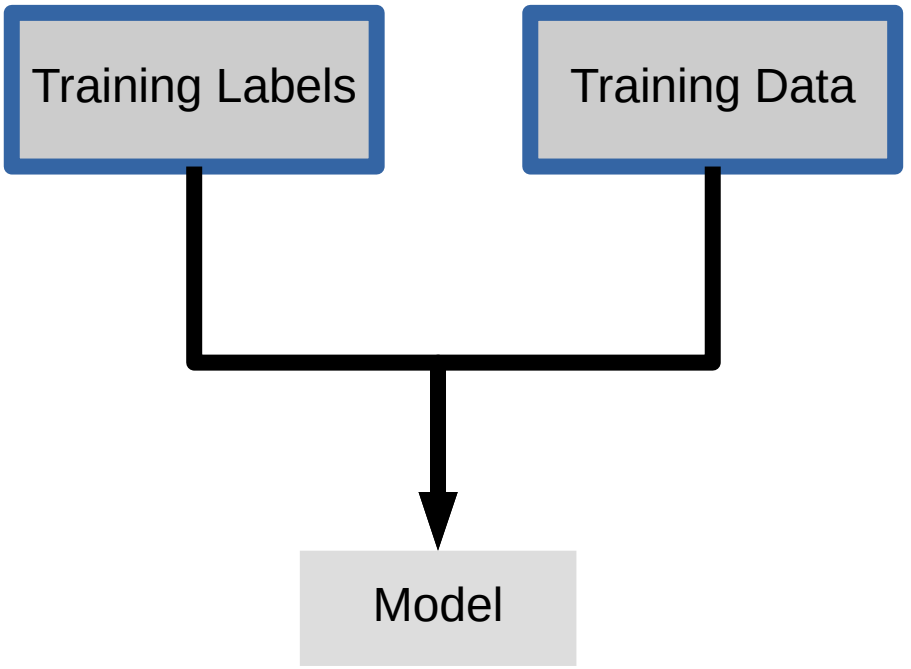
Cross-Validation

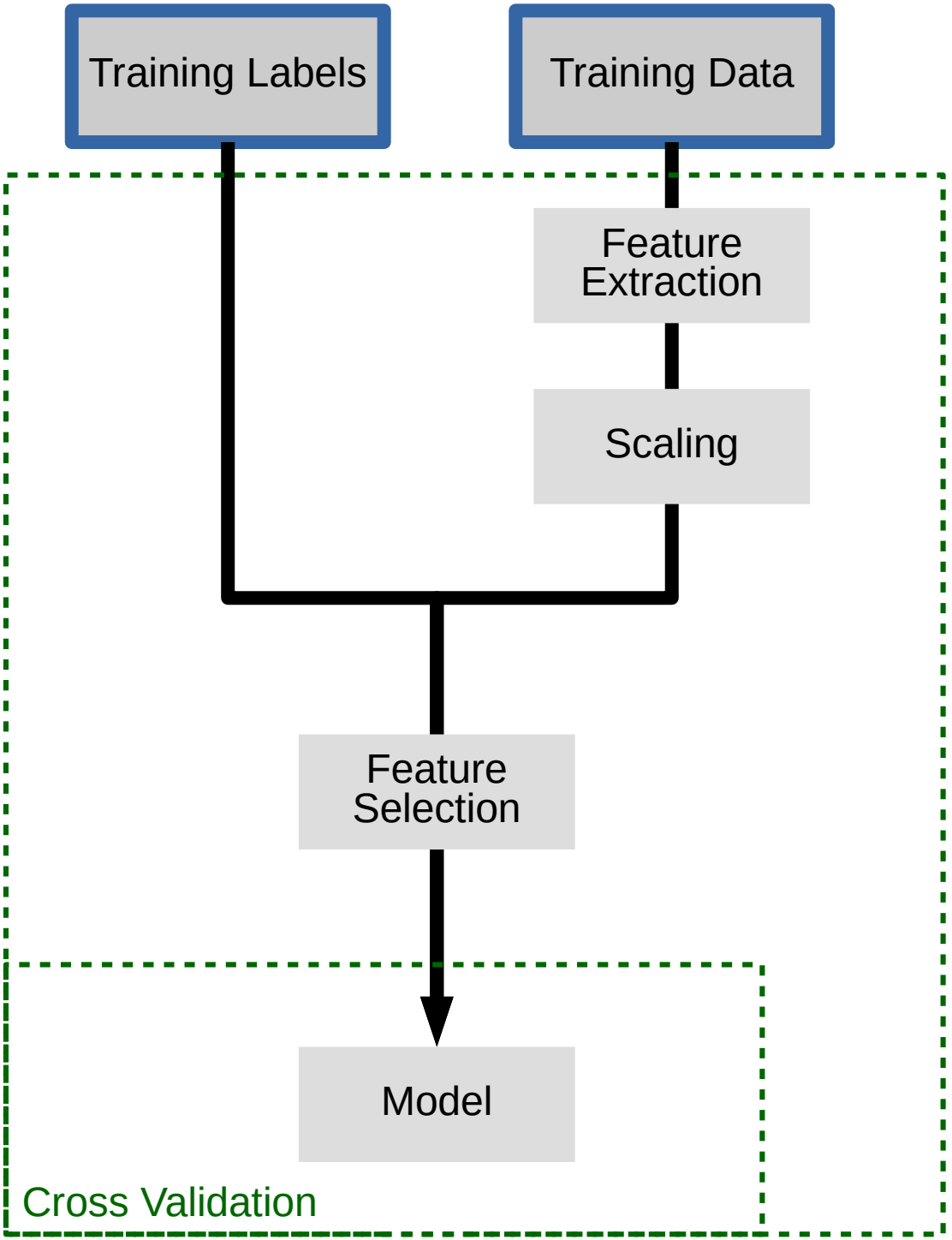
```
from sklearn.model_selection import cross_val_score
scores = cross_val_score(SVC(), X, y, cv=5)
print(scores)
>> [ 0.92  1.    1.    1.    1.  ]
```


All Data
Training data
Test data
Fold 1
Fold 2
Fold 3
Fold 4
Fold 5
Split 1
Split 2
Split 3
Split 4
Split 5
Finding Parameters
Final evaluation
Test data

Cross -Validated Grid Search

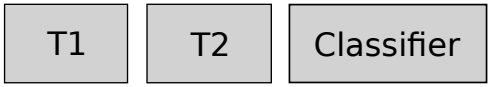
```
from sklearn.model_selection import GridSearchCV
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y)

param_grid = {'C': 10. ** np.arange(-3, 3),
              'gamma': 10. ** np.arange(-3, 3)}
grid = GridSearchCV(SVC(), param_grid=param_grid)
grid.fit(X_train, y_train)
grid.predict(X_test)
grid.score(X_test, y_test)
```


Training Labels
Training Data
Model

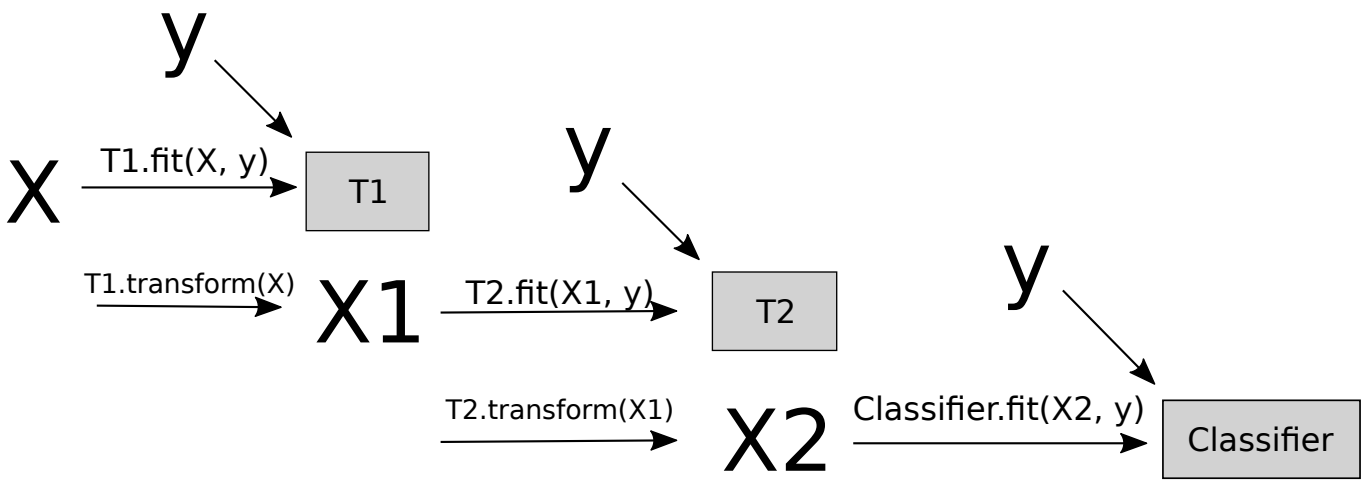

Training Labels
Training Data
Feature Extraction
Scaling
Feature Selection
Model
Cross Validation

Pipelines

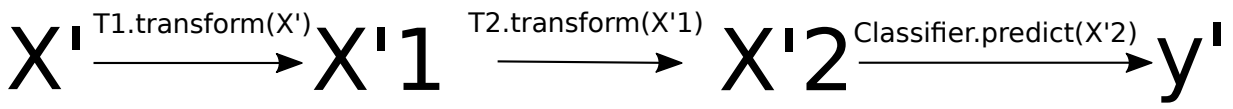
```
pipe = make_pipeline(T1(), T2(), Classifier())
```




```
pipe.fit(X, y)
```




```
pipe.predict(X')
```



Pipelines

```
from sklearn.pipeline import make_pipeline

pipe = make_pipeline(StandardScaler(), SVC())
pipe.fit(X_train, y_train)
pipe.predict(X_test)
```

```
param_grid = {'svc__C': 10. ** np.arange(-3, 3),
              'svc__gamma': 10. ** np.arange(-3, 3)}

scaler_pipe = make_pipeline(StandardScaler(), SVC())
grid = GridSearchCV(scaler_pipe, param_grid=param_grid, cv=5)
grid.fit(X_train, y_train)
```

Combining Pipelines and Grid Search

Proper cross-validation

```
param_grid = {'svc__C': 10. ** np.arange(-3, 3),
              'svc__gamma': 10. ** np.arange(-3, 3)}

scaler_pipe = make_pipeline(StandardScaler(), SVC())
grid = GridSearchCV(scaler_pipe, param_grid=param_grid, cv=5)
grid.fit(X_train, y_train)
```

Combining Pipelines and Grid Search II

Searching over parameters of the preprocessing step

```
param_grid = {'selectkbest__k': [1, 2, 3, 4],
              'svc__C': 10. ** np.arange(-3, 3),
              'svc__gamma': 10. ** np.arange(-3, 3)}

scaler_pipe = make_pipeline(SelectKBest(), SVC())
grid = GridSearchCV(scaler_pipe, param_grid=param_grid, cv=5)
grid.fit(X_train, y_train)
```

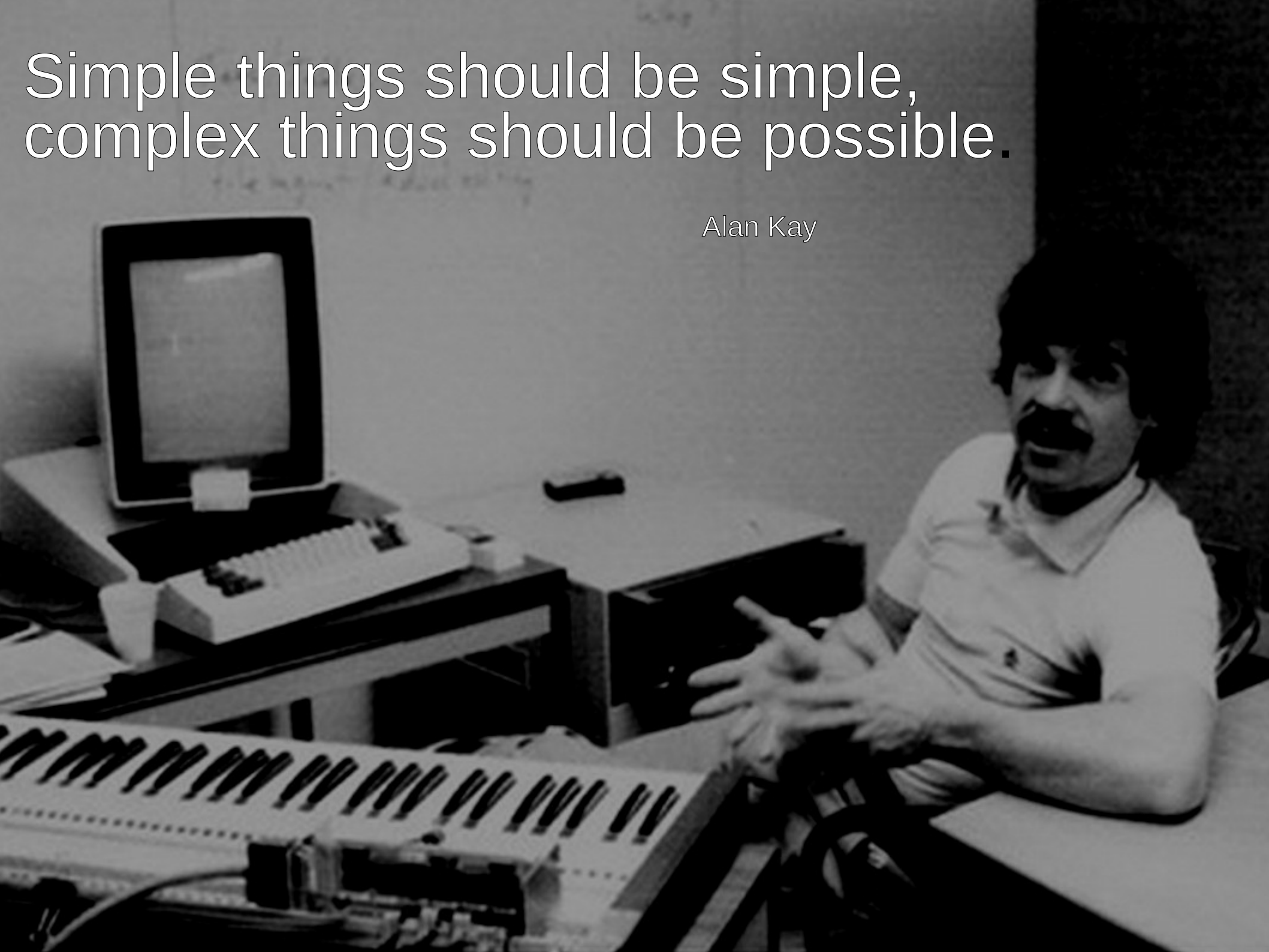
More API

Scorers

```
grid = GridSearchCV(SVC(), params, scoring='roc_auc')

def my_acc_scorer(est, X, y):
    y_pred = est.predict(X)
    return (y == y_pred).mean()

grid = GridSearchCV(SVC(), params,
                                scoring=my_acc_scorer)
```

Cross-validation iterators

```
grid = GridSearchCV(SVC(), param_grid, cv=5)

cv = KFold(n_split=5, shuffle=True, random_state=3)

grid = GridSearchCV(SVC(), param_grid, cv=cv)


cv = RepeatedKFold(n_split=5, n_repeats=10)
grid = GridSearchCV(SVC(), param_grid, cv=cv)
```


Simple things should be simple,
complex things should be possible.
Alan Kay

Simplicity

```
lr = LogisticRegression()
lr.fit(X_train, y_train)
lr.score(X_test, y_test)
```

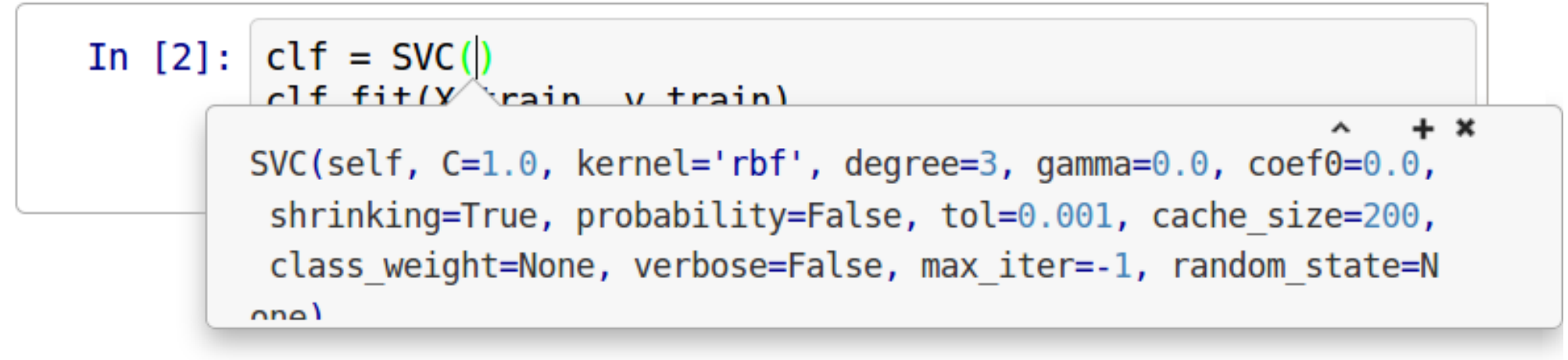
Consistency

```
grid = GridSearchCV(svm,param_grid)
grid.fit(X_train, y_train)
grid.score(X_test, y_test)
```

Composition

```
feature_selection = RFECV(NaiveBayes())
pipe = make_pipeline(feature_selection,
                     RandomForestClassifier())
grid = GridSearchCV(pipe, param_grid)
```

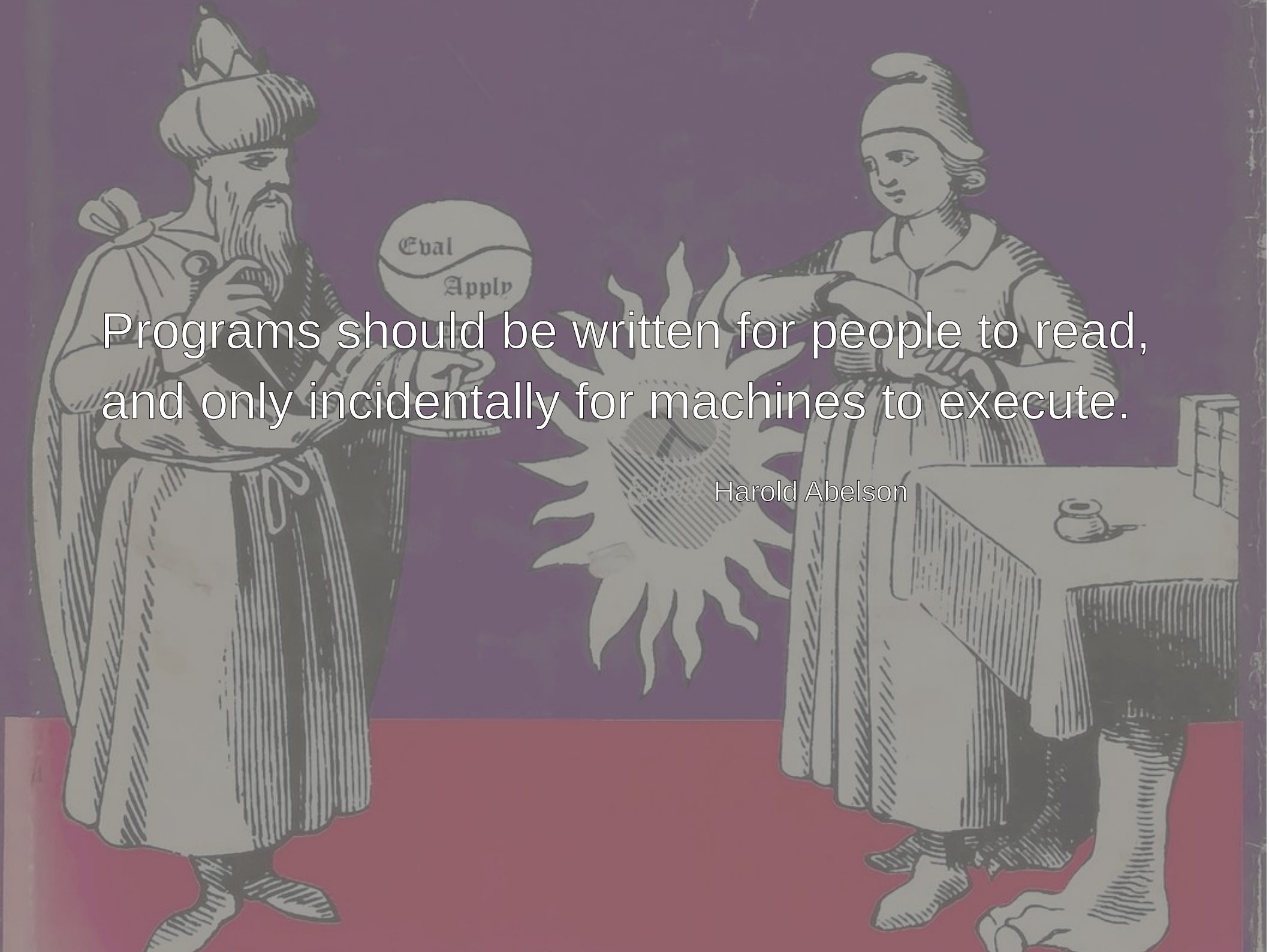
Default Parameters



Flat Class Hierarchy, Few Types

- Numpy arrays / sparse matrices
- Estimators
- Cross-validation objects
- Scorers

Development Practices



Programs should be written for people to read, and only incidentally for machines to execute.

Harold Abelson

Standards for OSS

Everything discussed in the open.
Every convention and process documented.

Development guide

http://scikit-learn.org/dev/developers/contributing.html

Contains:

- API details
- Bug report guidelines
- PR guidelines
- Reviewing guidelines
- How to find issues
- Details of CI

Even more at http://scikit-learn.org/dev/developers/

Deprecations / backward compatibility

- Don’t change any behavior (except bug fixes)

```
@property
@deprecated("Attribute labels_ was deprecated in version 0.13 and "
            "will be removed in 0.15. Use 'classes_' instead")
def labels_(self):
    return self.classes_
```

check_estimator

```python
class TemplateClassifier(BaseEstimator, ClassifierMixin):

    def __init__(self, demo_param='demo'):
        self.demo_param = demo_param

    def fit(self, X, y):

        # Check that X and y have correct shape
        X, y = check_X_y(X, y)
        # Store the classes seen during fit
        self.classes_ = unique_labels(y)

        self.X_ = X
        self.y_ = y
        # Return the classifier
        return self

    def predict(self, X):

        closest = np.argmin(euclidean_distances(X, self.X_), axis=1)
        return self.y_[closest]
```

```
check_estimator(TemplateClassifier)
```

```
AssertionError: Error message does not include the expected string: 'fit'.
Observed error message: "'TemplateClassifier' object has no attribute 'X_'"
```

Coming up for 0.20
(July / August 2018)

ColumnTransformer

```
# We create the preprocessing pipelines for both numeric and categorical data.
numeric_transformer = make_pipeline(SimpleImputer(), StandardScaler())
categorical_transformer = CategoricalEncoder('onehot-dense',
                                              handle_unknown='ignore')

preprocessing_pl = make_column_transformer(
    (numeric_features, numeric_transformer),
    (categorical_features, categorical_transformer),
    remainder='drop'
)

# Append classifier to preprocessing pipeline.
# Now we have a full prediction pipeline.
clf = make_pipeline(preprocessing_pl, LogisticRegression())
```

OneHotEncoder for Strings

```
>>> from sklearn.preprocessing import OneHotEncoder
>>> enc = OneHotEncoder(handle_unknown='ignore')
>>> X = [['Male', 1], ['Female', 3], ['Female', 2]]
>>> enc.fit(X)
...
OneHotEncoder(categorical_features=None, categories=None,
       dtype=<... 'numpy.float64'>, handle_unknown='ignore',
       n_values=None, sparse=True)
```

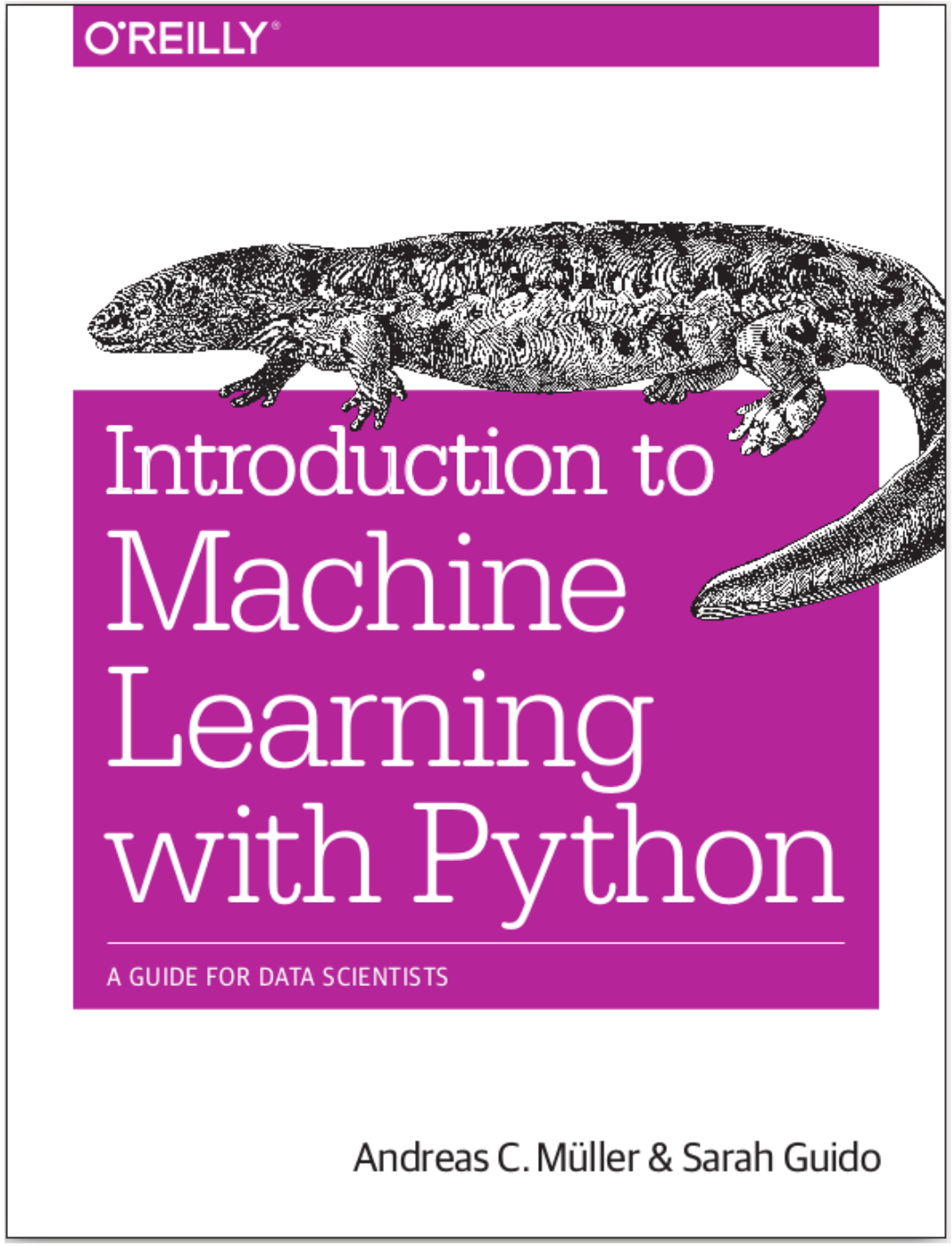
```
>>> enc.categories_
[array(['Female', 'Male'], dtype=object), array([1, 2, 3], dtype=object)]
>>> enc.transform([['Female', 1], ['Male', 4]]).toarray()
array([[1., 0., 1., 0., 0.],
       [0., 1., 0., 0., 0.]])
>>> enc.inverse_transform([[0, 1, 1, 0, 0], [0, 0, 0, 1, 0]])
array([['Male', 1],
       [None, 2]], dtype=object)
```

NaN handling in Scalers
Better imputation

(my personal) Roadmap

Make simple things simple again!

Pandas Integration
Feature Names
More convenient preprocessing
Plotting Tools
Estimator Tags



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